A Coupling Tool for Parallel Molecular Dynamics–Continuum Simulations

ISPDC 2012

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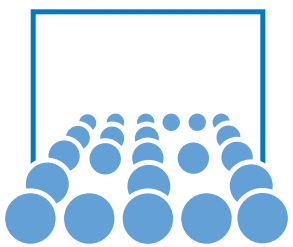
29.06.2012



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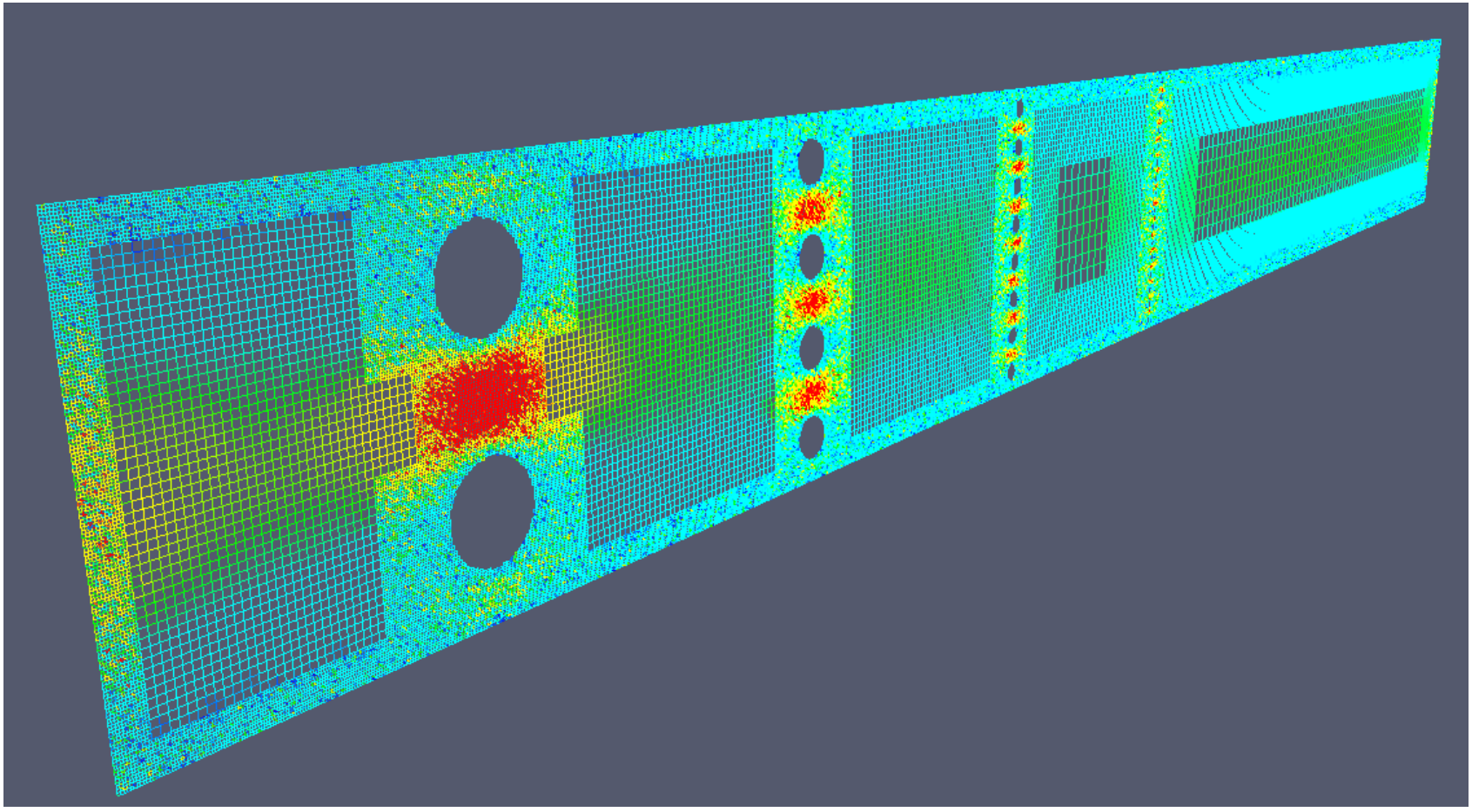
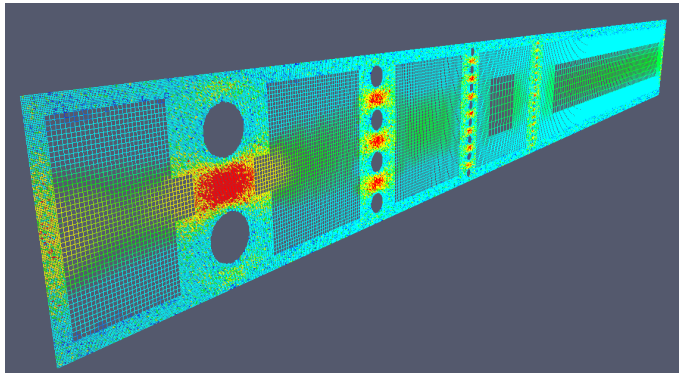
Hybrid Molecular–Continuum Simulations: Why?



Hybrid Molecular–Continuum Simulations: Why?

- Huge interest in flows at micro- to nanoscale
  $\rightarrow$ Biosensors, micropumps, ...
- Nanoflows: May represent only small part of huge flow system



- Molecular Dynamics (MD) required to capture correct flow behaviour

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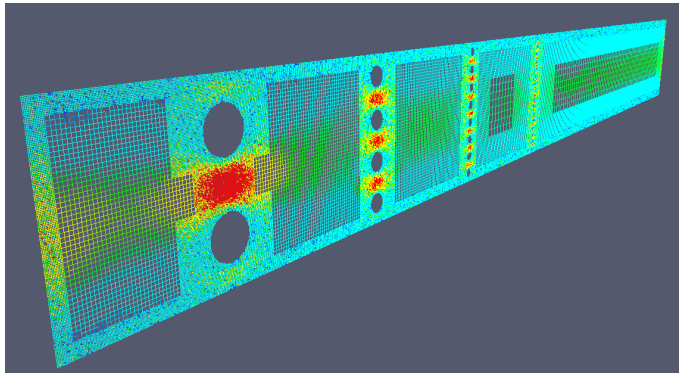
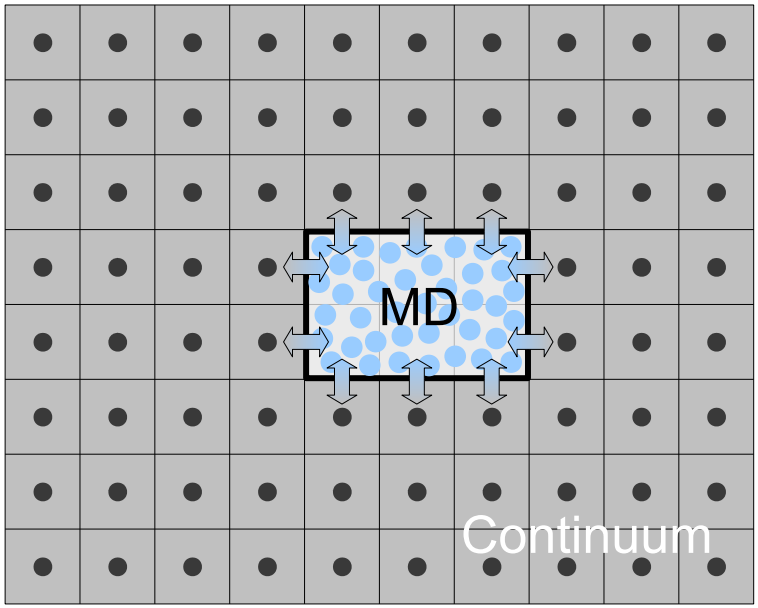
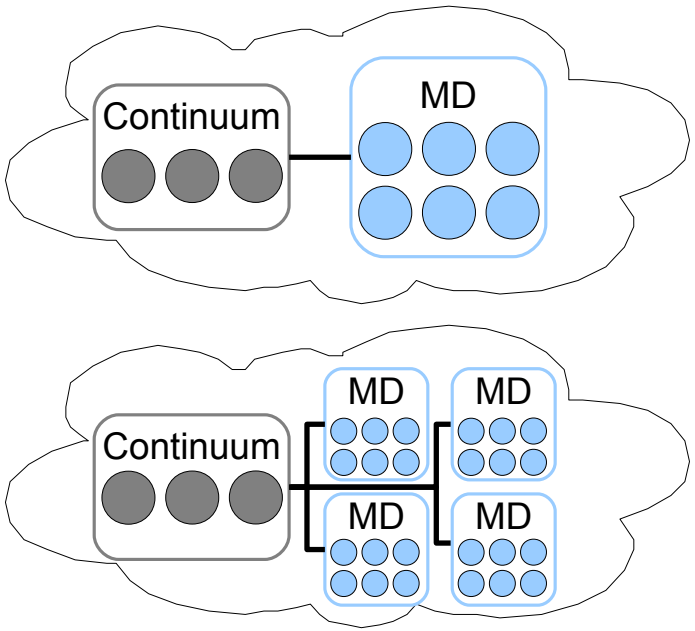


- Molecular Dynamics (MD) required to capture correct flow behaviour

Computationally expensive accurate MD simulations $\Leftrightarrow$ Less accurate computationally cheap continuum simulations

Challenges: Physics & Distributed Computing





- Correct physical description at molecular–continuum interface
- Simple & fast testing of new coupling schemes

- Statistical noise on MD data [3] $\rightarrow$ sampling
- Flexibility
- (Massively) Parallel implementation

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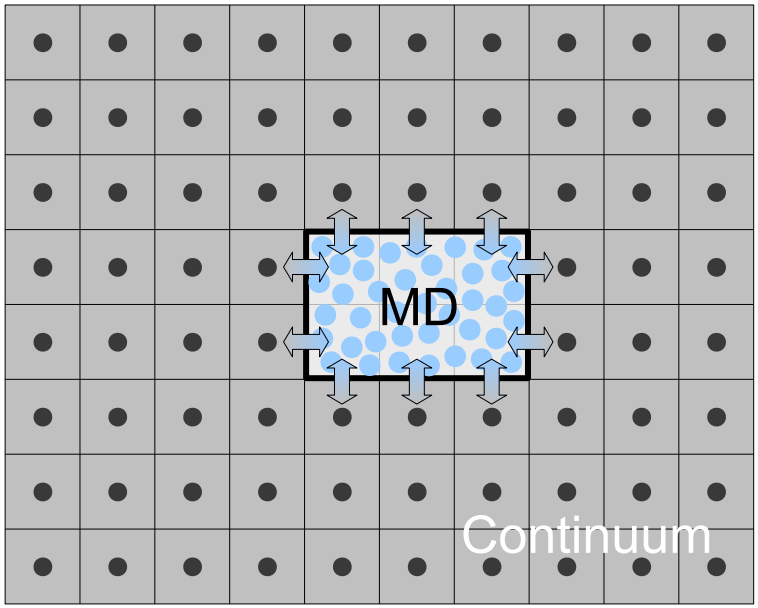

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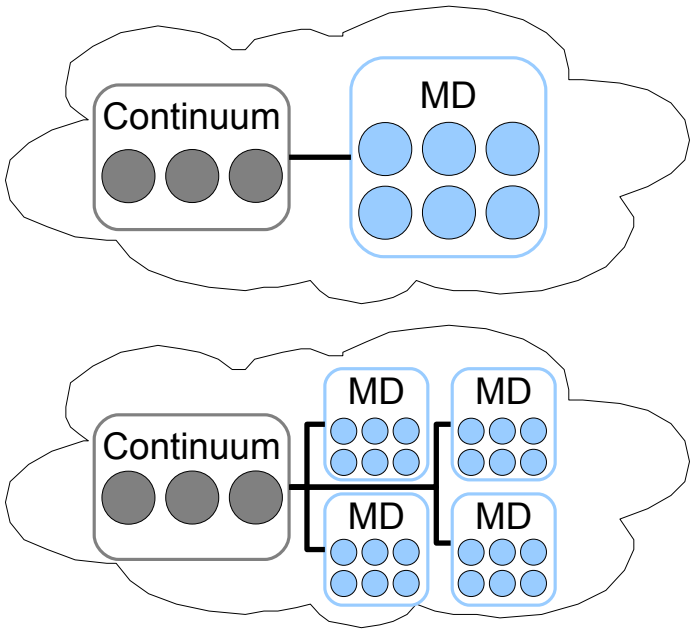

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Macro–Micro Coupling: Preparations

MD → Continuum:

Mass exchange	→	average number of molecules
Momentum exchange	→	average velocities/ momentum of molecules
Energy exchange		

Continuum → MD:

Mass exchange	→	insert/ delete molecules
Momentum exchange	→	in-/ decrease velocities of molecules
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Molecular Dynamics

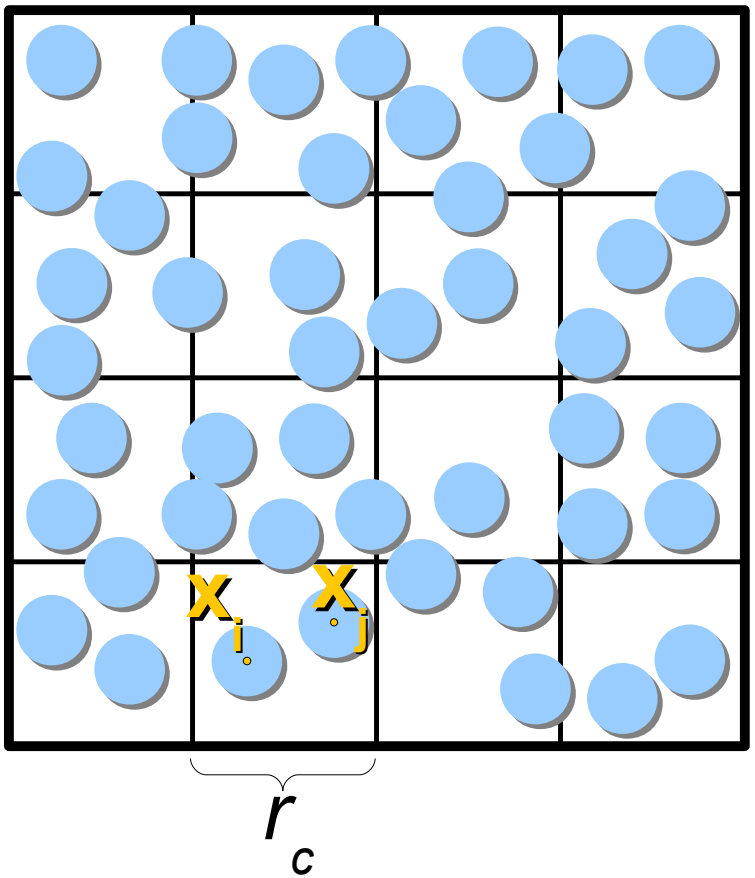
- Linked-Cell-based MD simulations
- (Truncated Shifted) 12-6 Lennard Jones potential

$$U_{LJ}^{cut}(\|\mathbf{r}_{ij}\|) := U_{LJ}(\|\mathbf{r}_{ij}\|) - U_{LJ}(r_c)$$

where

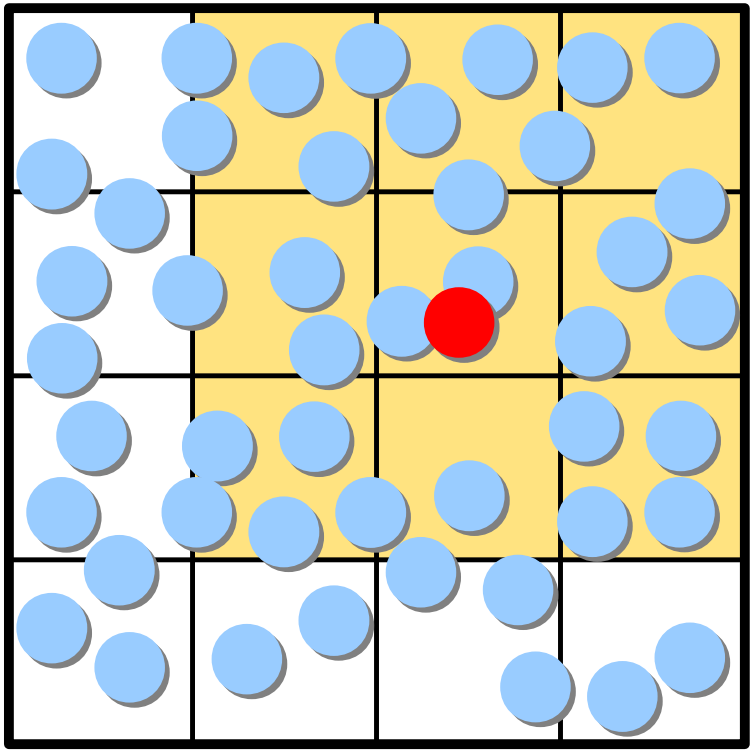
$$U_{LJ}(r) := 4\epsilon \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right),$$

$\mathbf{r}_{ij} := \mathbf{x}_j - \mathbf{x}_i$ and r_c cut-off radius



Particle Insertion

Goal: Insert particle with potential energy U_{pot} close to prescribed target energy U_{target}



USHER-Algorithm [2]:

1. Choose random position
2. Evaluate potential energy U_{pot}
3. If ($U_{pot} - U_{target} <$ TOL) return;
4. Move particle towards U_{target}; Go to **1.**

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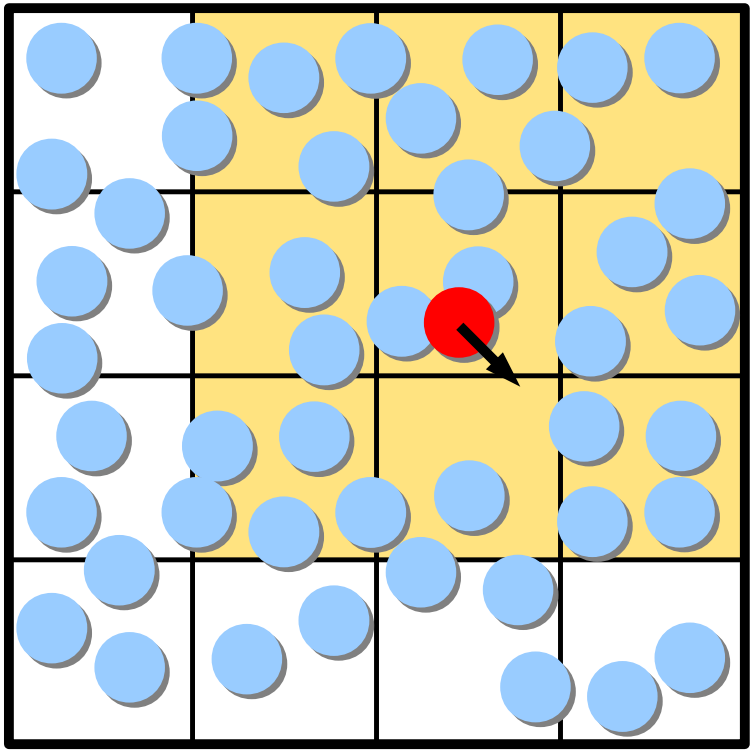

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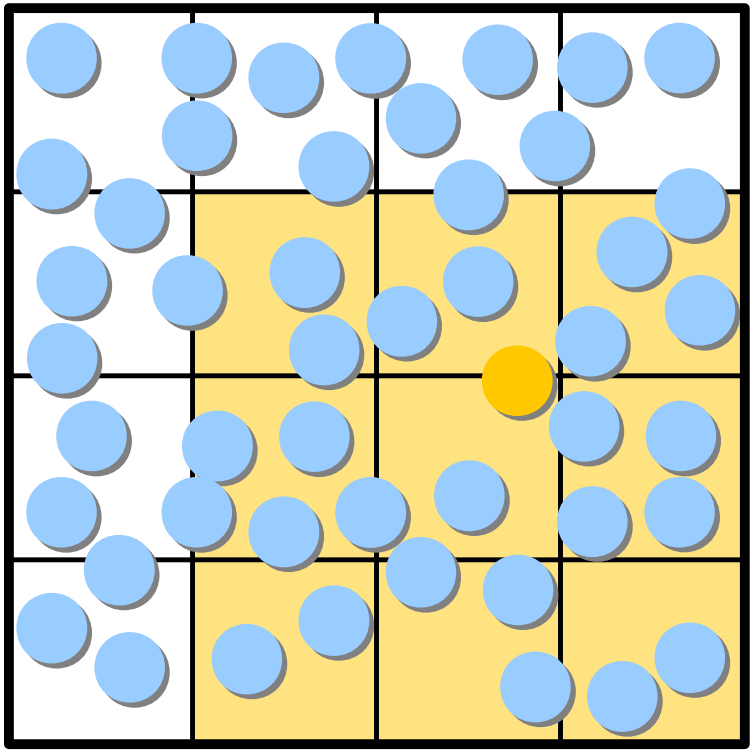

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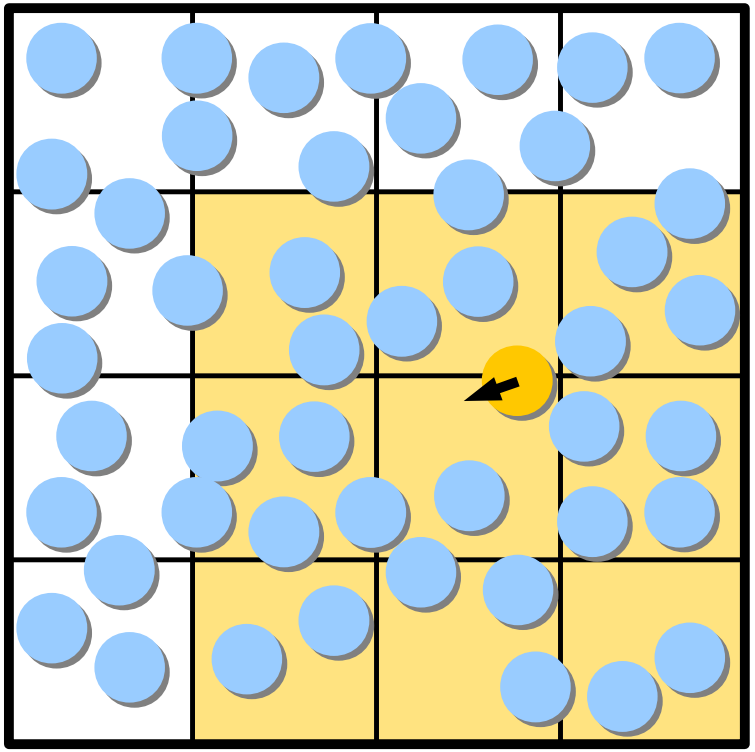

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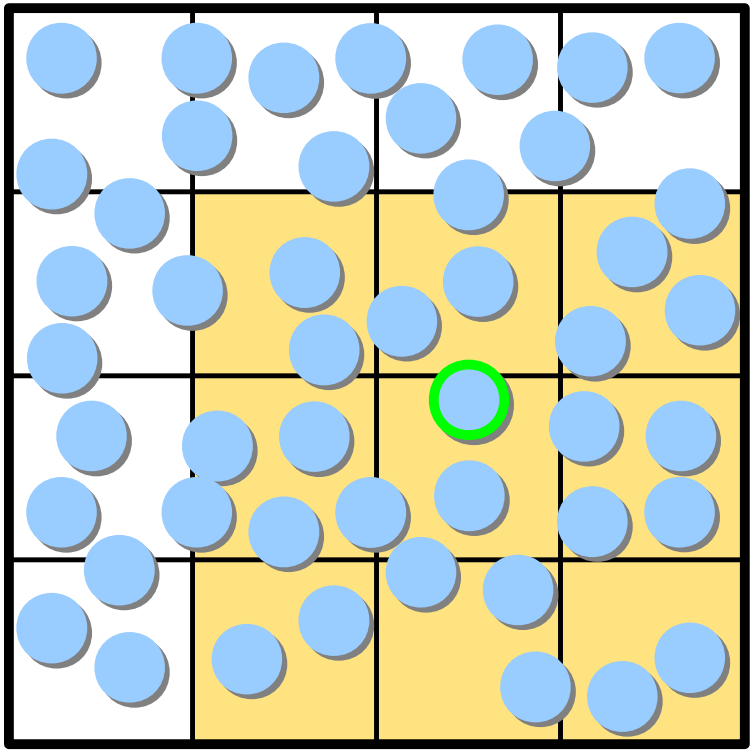

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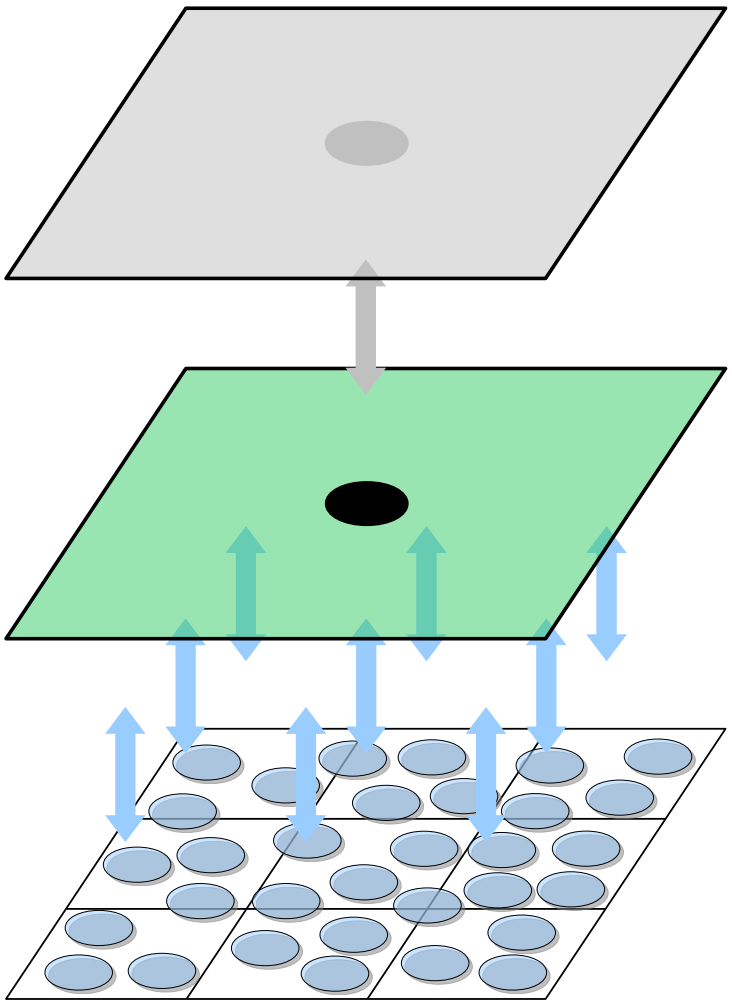
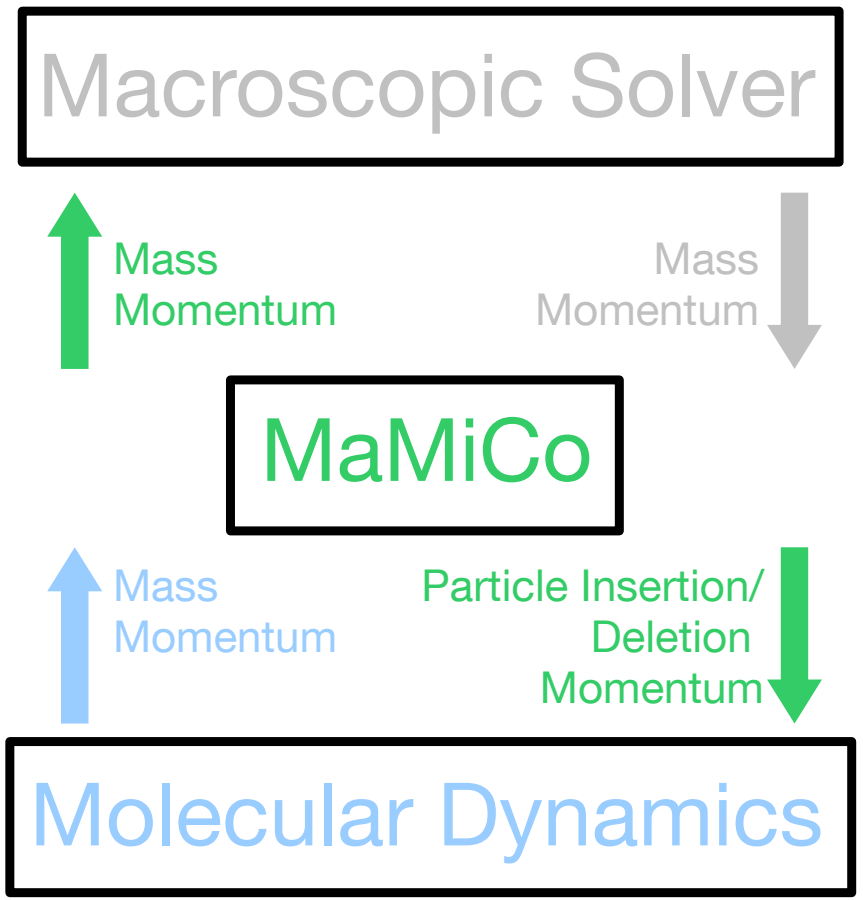
The Macro–Micro Coupling Tool (MaMiCo)





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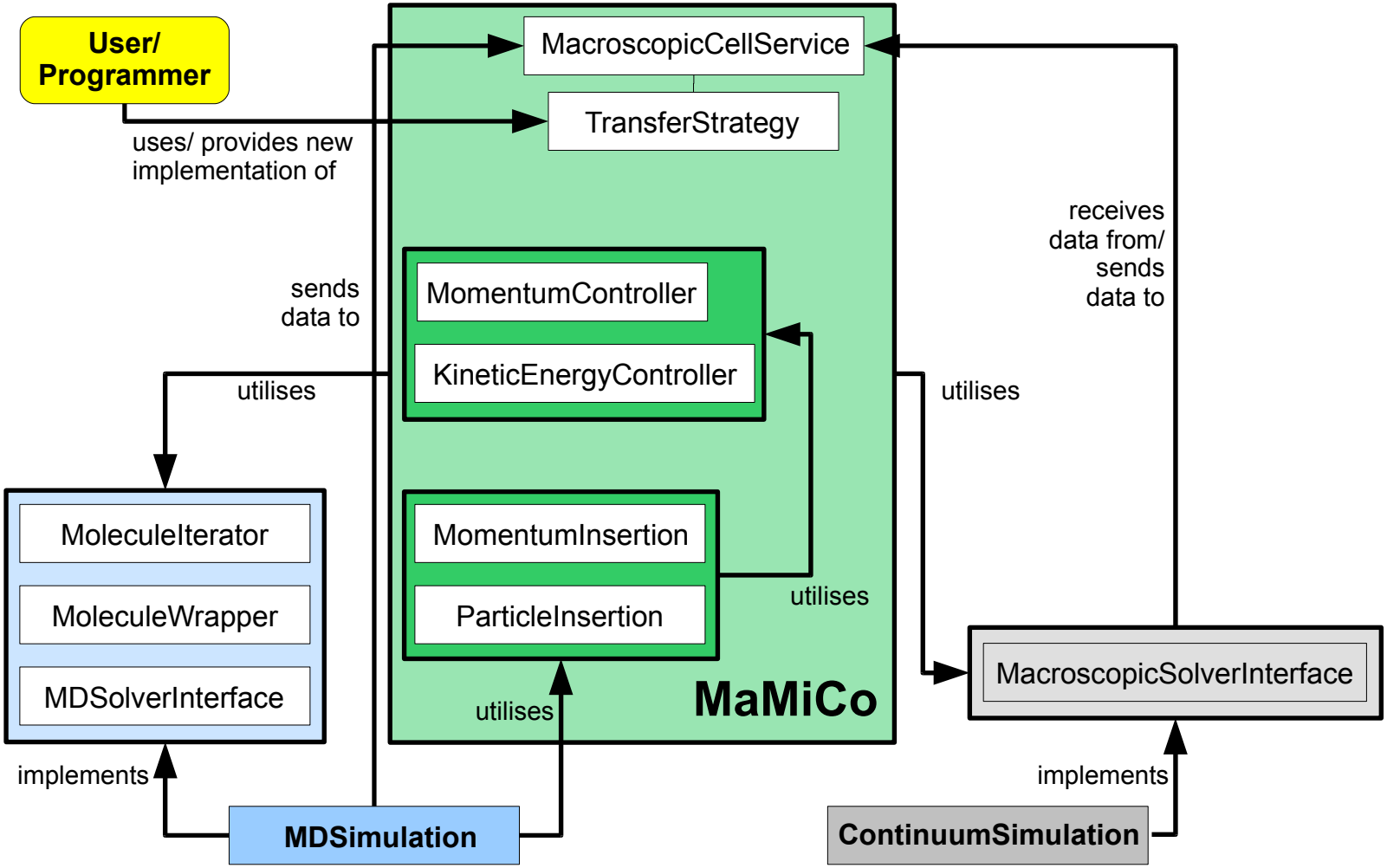
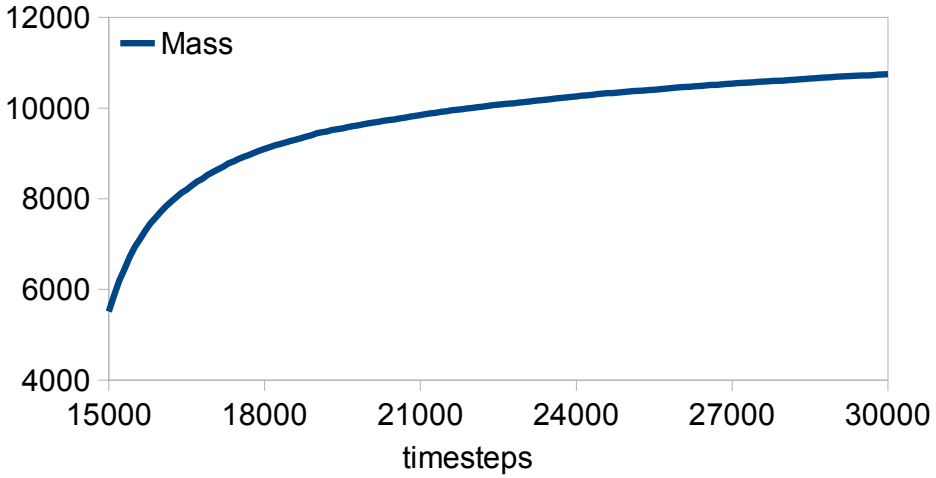
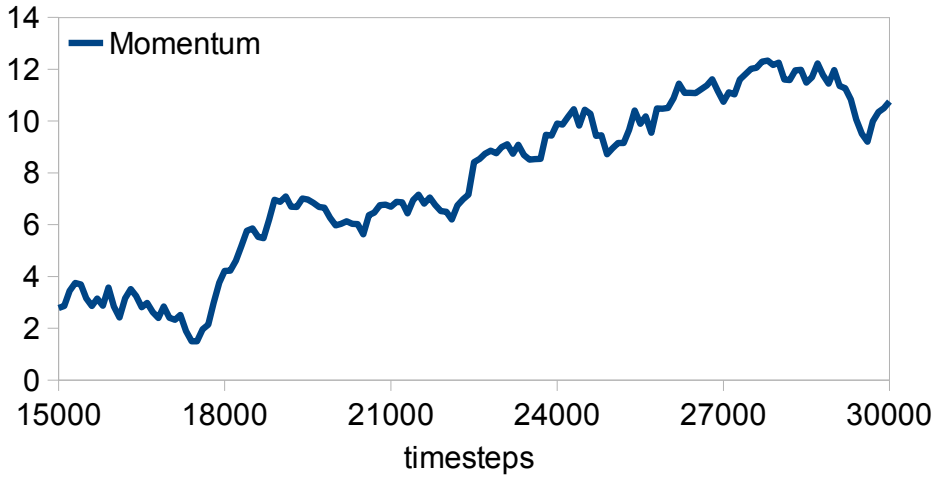
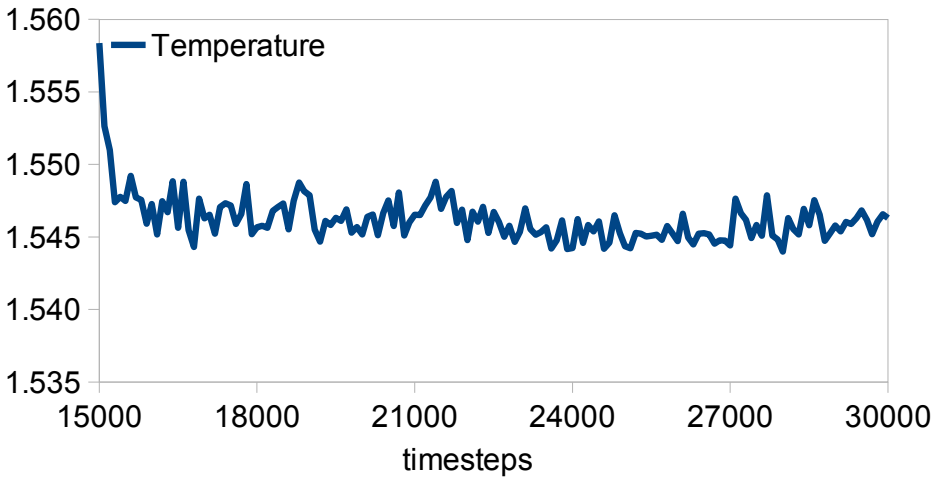


Validation: Mass insertion (1)







- Equilibrate MD system
- Double number of molecules
- Keep momentum and temperature constant

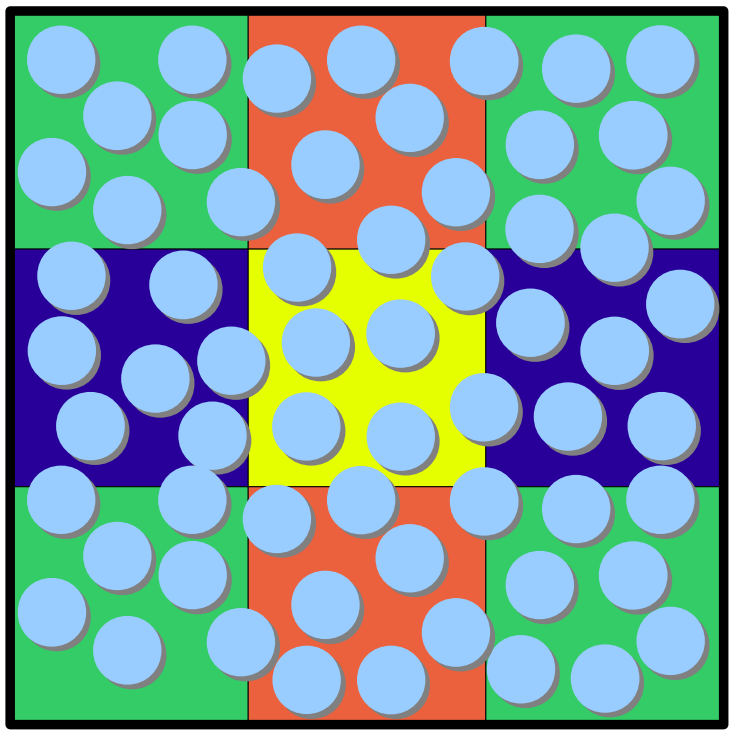
Validation: Mass insertion (2)

Scenario	Runtime (s)	Timesteps/ Particle insertion	Timesteps/ Momentum insertion
MD($n = 0.40$) (2D)	23.5	0	0
MD($n = 0.78$) (2D)	46.6	0	0
Test A (2D)	55.9	30	0
MD($n = 0.80$) (2D)	48.0	0	0
Test B ($n = 0.80$) (2D)	54.8	0	30
MD($n = 0.40$) (3D)	92.1	0	0
MD($n = 0.78$) (3D)	166.7	0	0
Test A (3D)	268.4	15	0
MD($n = 0.80$) (3D)	167.7	0	0
Test B ($n = 0.80$) (3D)	175.2	0	15

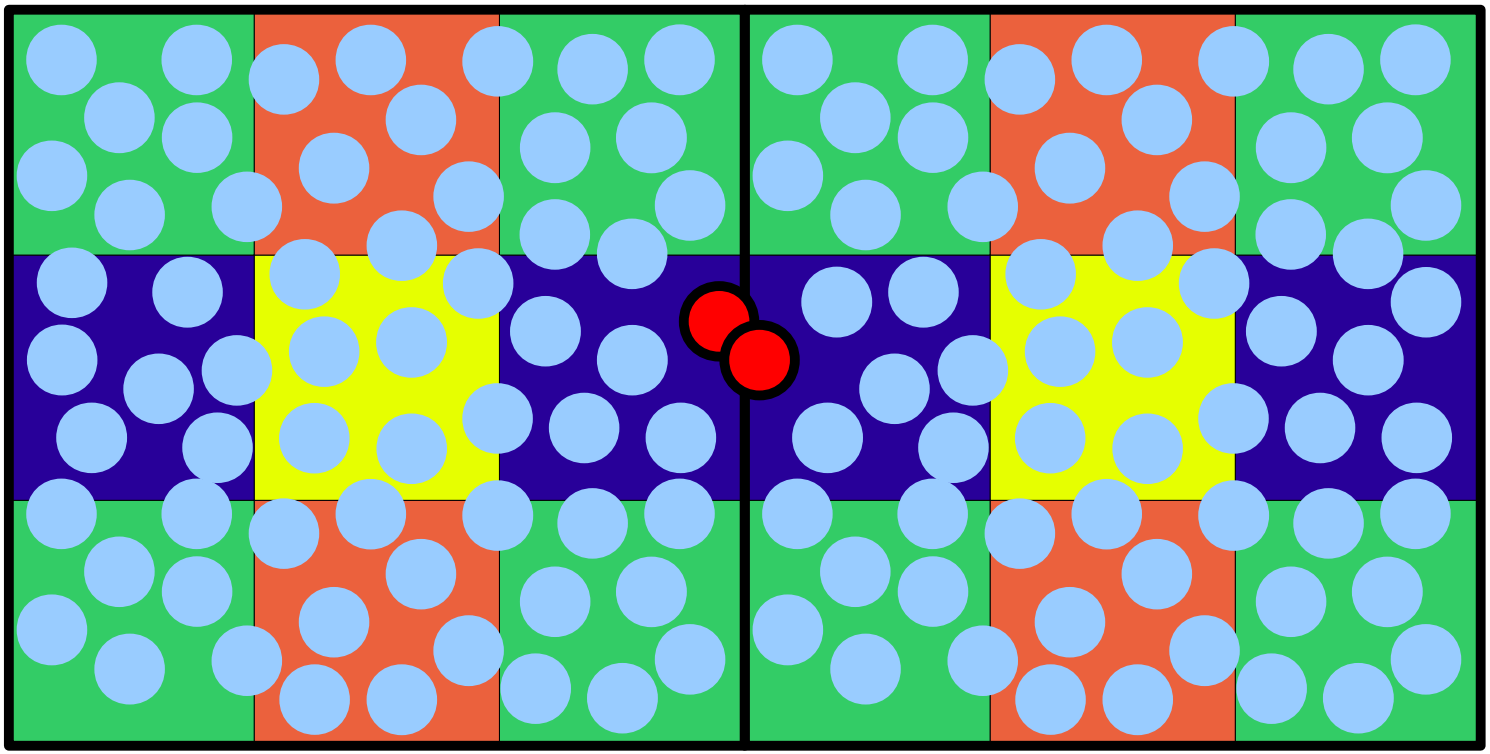
Parallel Particle Insertion (1)

2^D-**cell colouring**:

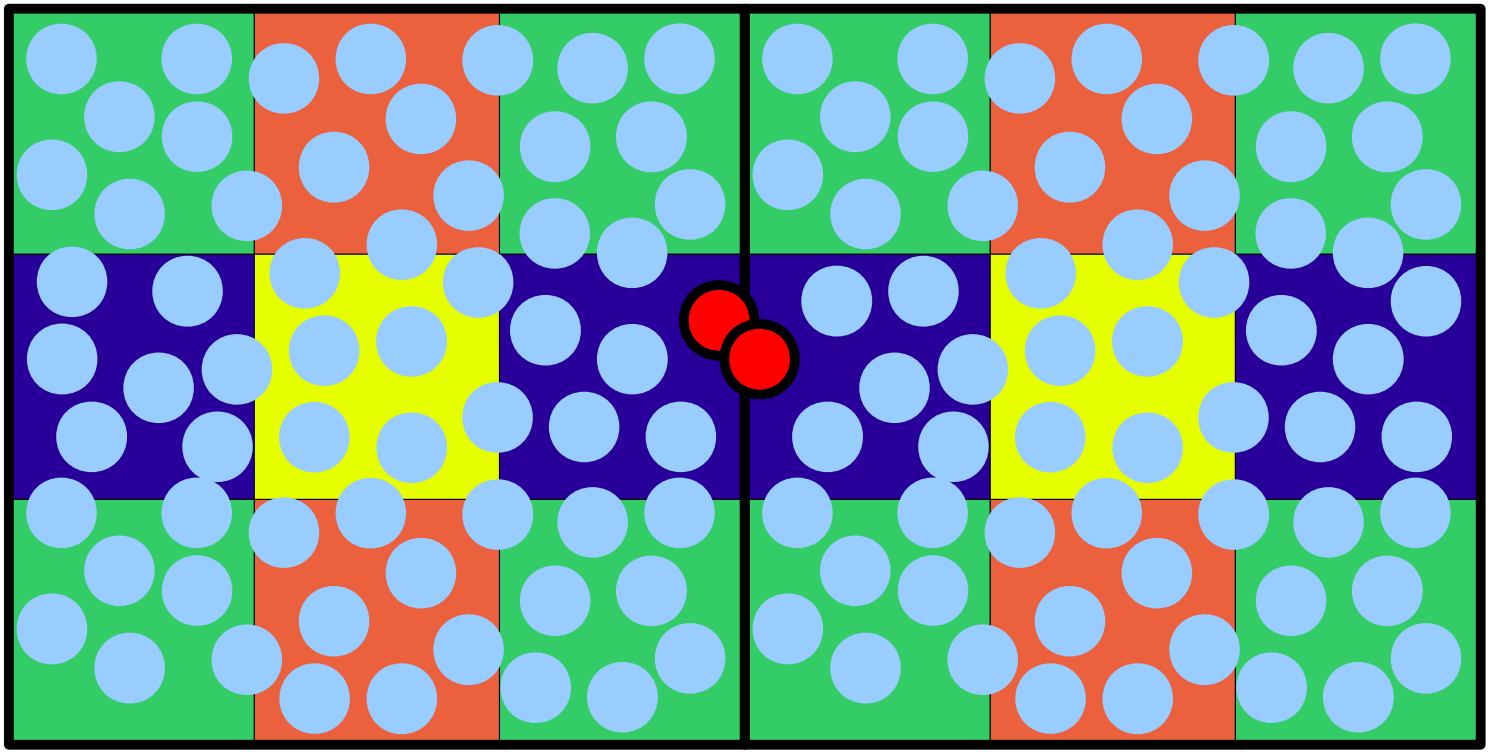
- Setup of potential energy landscape
- Standard approach for shared memory parallelisation



Parallel Particle Insertion (2)



Parallel Particle Insertion (2)



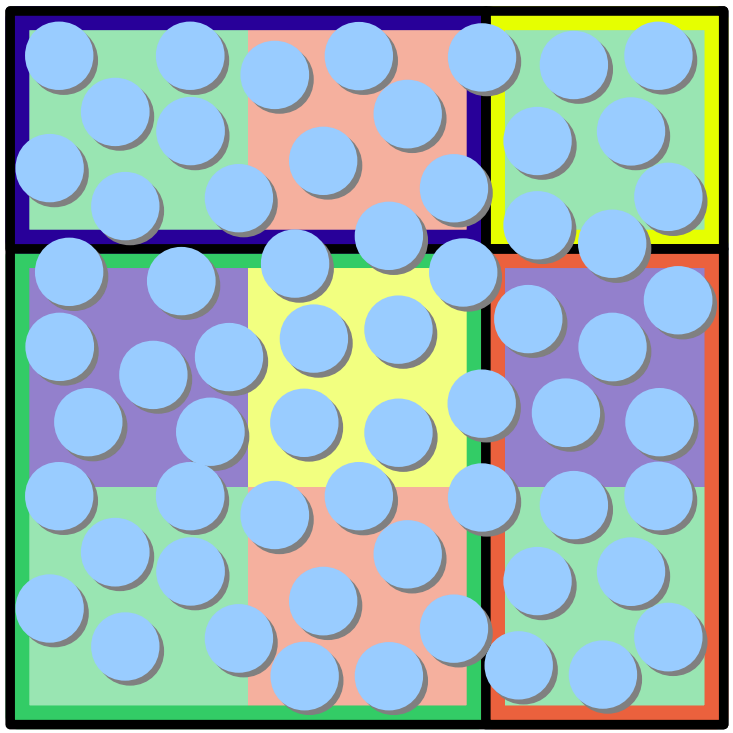
Conflicts in case of

- distributed memory parallelisation
- periodic boundaries

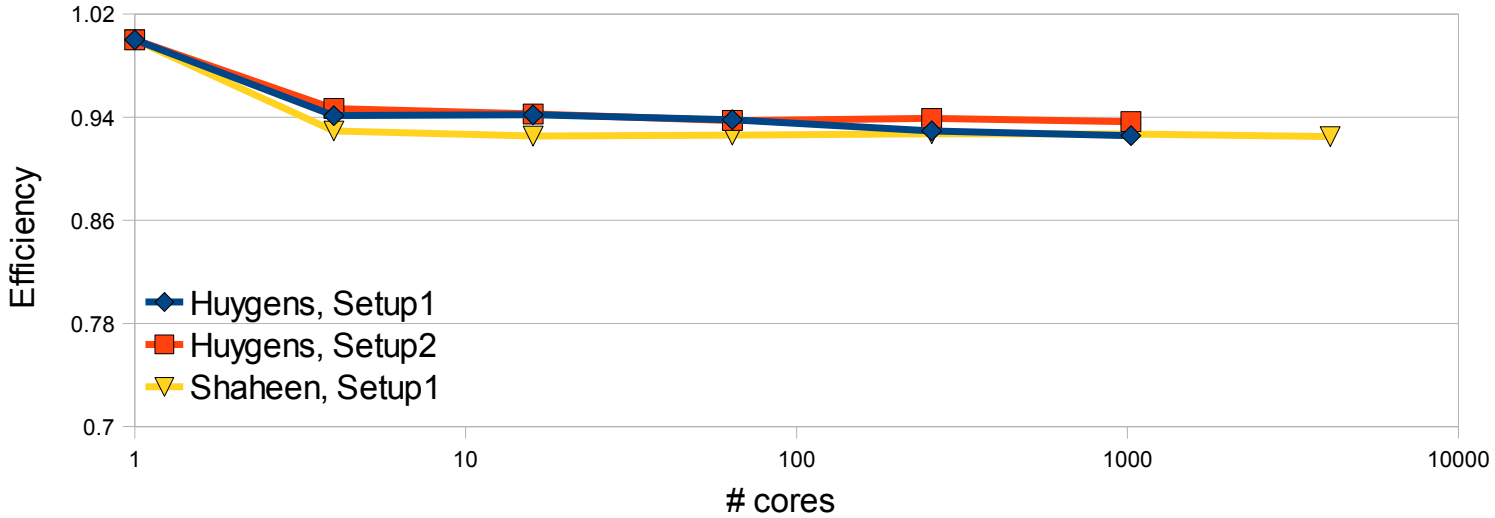
Parallel Particle Insertion (3)

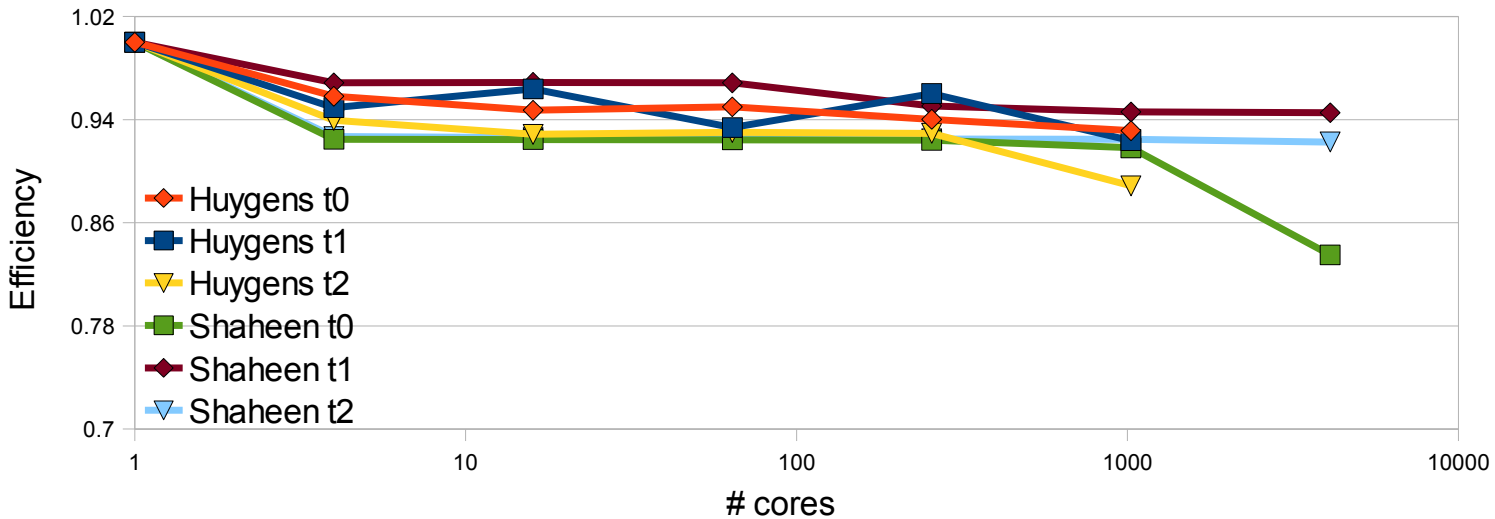
2^D-**block colouring** [1]:

- Resolves conflict across processes
- Inside each block: cell-colouring

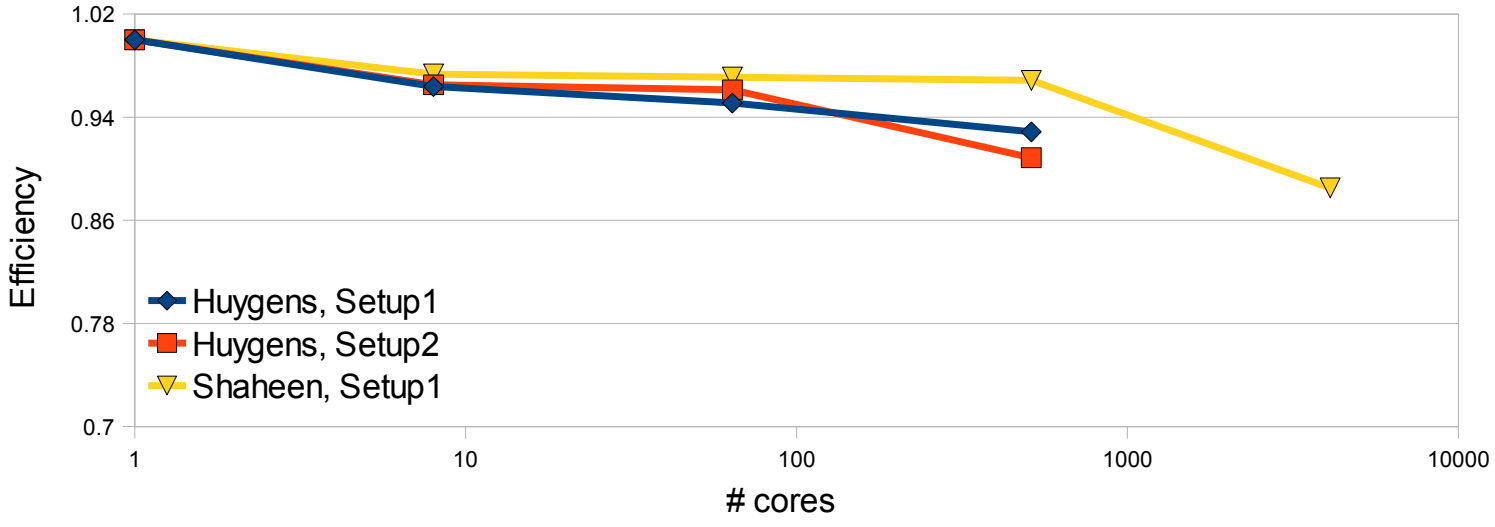


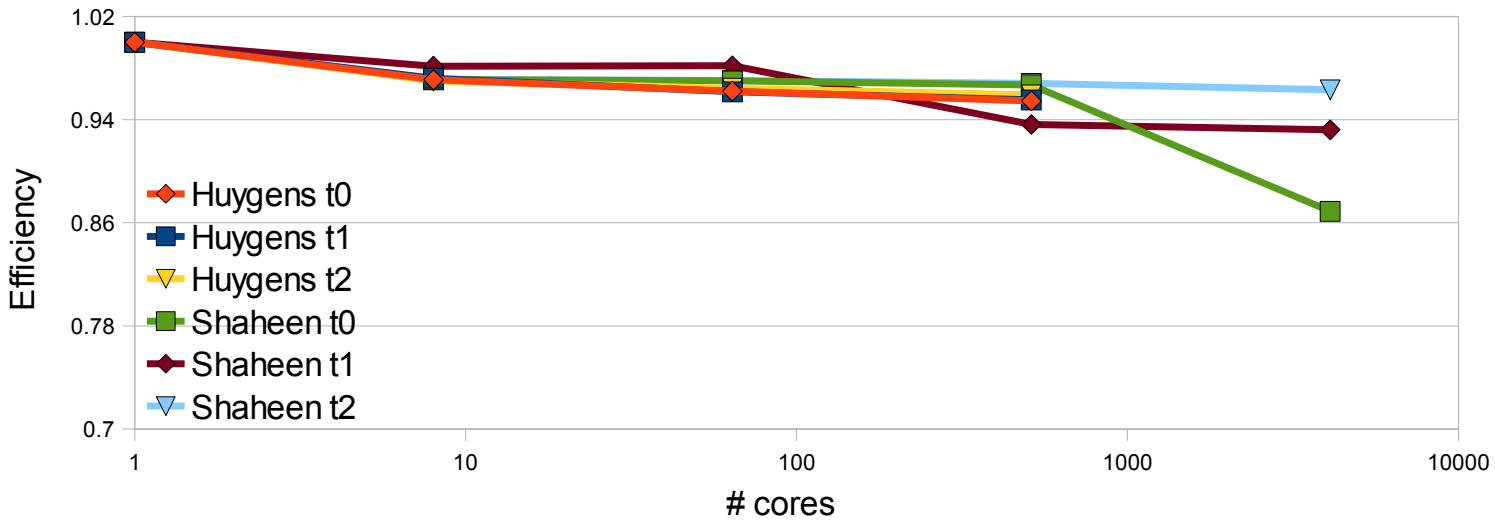
Parallel Particle Insertion: Results (2D)





Parallel Particle Insertion: Results (3D)





Conclusion & Outlook

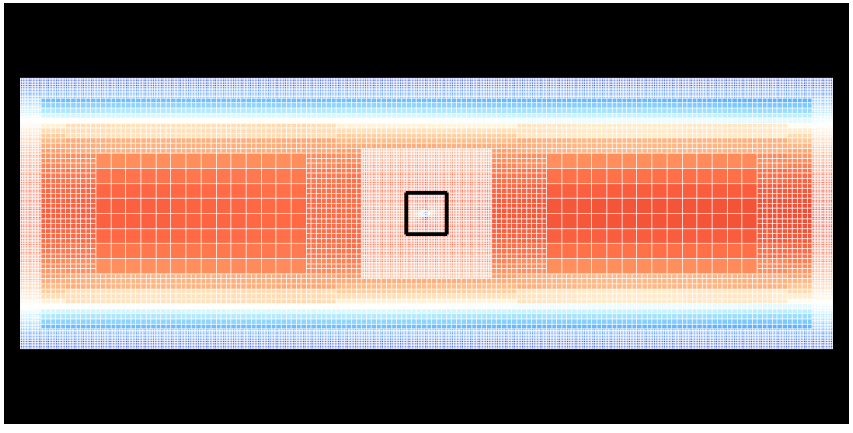
Conclusion:

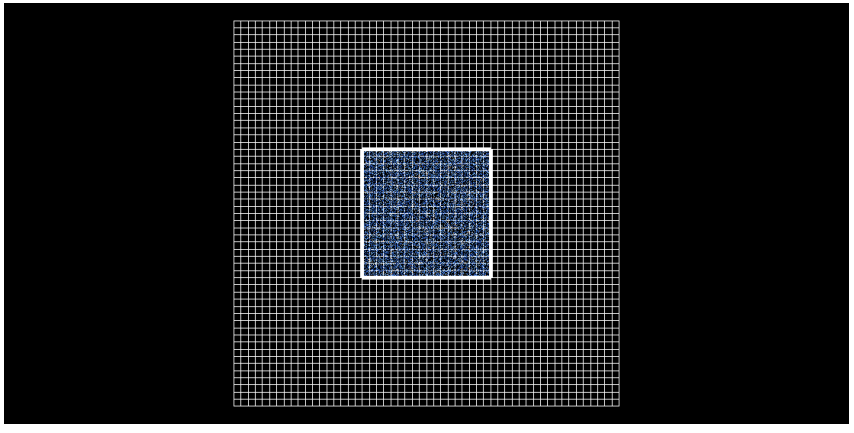
- Tool for hybrid molecular–continuum simulations (MaMiCo)
- 2D/ 3D support
- Distributed memory parallelisation: Particle insertions and more

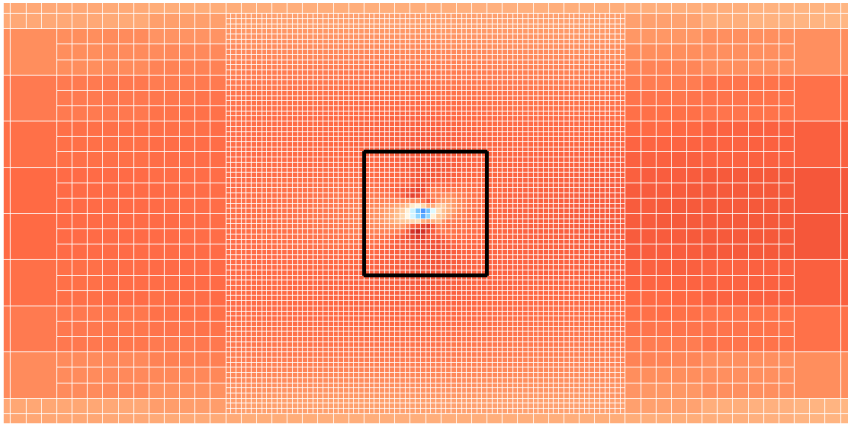
Outlook: From tests to parallel coupling algorithms

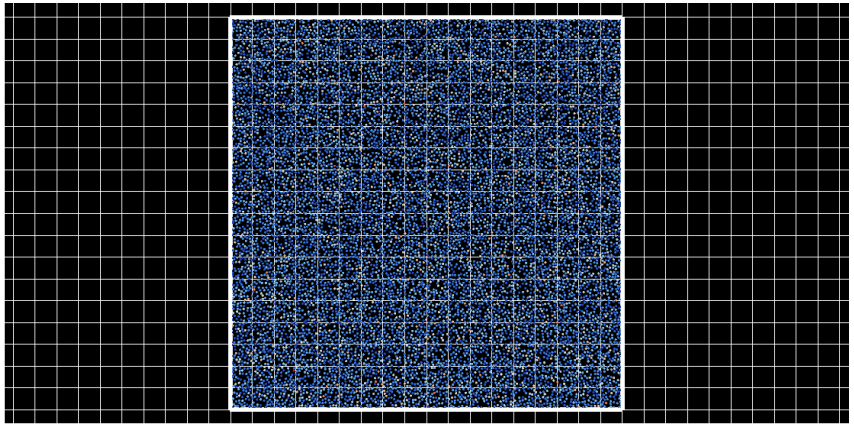
Spatially adaptive Lattice Boltzmann implementation	+	(Complex) Molecular Dynamics	=	

New Insights...









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